SO(4) symmetry and off-diagonal long-range order in the Hubbard bilayer

Short title: Hubbard bilayer

Yu Shi

Fudan-T. D. Lee Physics Laboratory and Department of Physics,

Fudan University, Shanghai 200433, People's Republic of China

Abstract

Yang's η pairing operator is generalized to explore off-diagonal long-range order in the Hubbard bilayer with an arbitrary chemical potential. With this operator and a constraint condition on annihilation and creation operators, we construct explicitly eigenstates which possess simultaneously three kinds of off-diagonal long-range order, i.e., the intralayer one and the interlayer one for on-site pairing, and that for interlayer nearest-neighbor pairing. As in the simple Hubbard model there is also an SO(4) symmetry, with the the generators properly defined. A sufficient condition leads to at least one of the above three kinds of off-diagonal long-range order. A constraint relation among different kinds of off-diagonal long-range order is also given. There exists a triplet of collective modes if the U(1) symmetry of a subgroup is spontaneously broken.

I. Introduction

Off-diagonal long-range order (ODLRO) is essential for the phenomena of superconductivity and superfluidity [1]. The BCS wave function does have ODLRO via cooper pairing [2], however, it is not an eigenstate of the Hamiltonian. In the search for the mechanism of high temperature superconductivity, the Hubbard model is studied intensively. Yang constructed explicitly many eigenstates, which is metastable for attractive interaction, of the Hubbard Hamiltonian possessing ODLRO [3]. Furthermore, Yang and Zhang uncovered an SO(4) symmetry and put forward a sufficient condition for any state to possess ODLRO [4]. Then Zhang predicted a triplet of collective modes, the massless Goldstone mode and a pair of massive modes, in the superconducting state [13].

In this paper we extend these discussions to the Hubbard bilayer, i.e., two Hubbard planes coupled by interlayer hopping. The motivation is that strong coupling between the adjacent CuO_2 planes of one double plane has been directly revealed experimently [5] [6][7][8]. The η pairing operator generalized from Yang's is introduced in Sec. II. Explicit eigenstates with ODLRO are constructed in Sec. III. SO(4) symmetry and the sufficient condition for a state to possess ODLRO is discussed in Sec. IV, where a constraint relation among different kinds of ODLRO is also given. In Sec. V, the triplet of collective modes are discussed. A brief summary is contained in Sec. VI, where some open problems are raised.

II. η pairing

The Hamiltonian is

$$
\begin{aligned}
H &= T_{\parallel}(A) + T_{\parallel}(B) + T_{\perp} + V, &(1)\\
T_{\parallel}(A) &= t_{\parallel}\sum_{r,\delta}(a^{\dagger}_{r\uparrow}a_{r+\delta\uparrow} + a^{\dagger}_{r\downarrow}a_{r+\delta\downarrow}),\\
&= \sum_{k}\epsilon(k)(a^{\dagger}_{k\uparrow}a_{k\uparrow} + a^{\dagger}_{k\downarrow}a_{k\downarrow}), &(2)\\
T_{\parallel}(B) &= t_{\parallel}\sum_{r,\delta}(b^{\dagger}_{r\uparrow}b_{r+\delta\uparrow} + b^{\dagger}_{r\downarrow}b_{r+\delta\downarrow})\\
&= \sum_{k}\epsilon(k)(b^{\dagger}_{k\uparrow}b_{k\uparrow} + b^{\dagger}_{k\downarrow}b_{k\downarrow}), &(3)\\
T_{\perp} &= t_{\perp}\sum_{r}(a^{\dagger}_{r\uparrow}b_{r\uparrow} + a^{\dagger}_{r\downarrow}b_{r\downarrow} + b^{\dagger}_{r\uparrow}a_{r\uparrow} + b^{\dagger}_{r\downarrow}a_{r\downarrow})\\
&= t_{\perp}\sum_{k}(e^{-iq_zd}a^{\dagger}_{k\uparrow}b_{k\uparrow} + e^{-iq_zd}a^{\dagger}_{k\downarrow}b_{k\downarrow} + e^{iq_zd}b^{\dagger}_{k\uparrow}a_{k\uparrow} + e^{iq_zd}b^{\dagger}_{k\downarrow}a_{k\downarrow}), &(4)\\
V &= U\sum_{r}[(a^{\dagger}_{r\uparrow}a_{r\uparrow} - \mu)(a^{\dagger}_{r\downarrow}a_{r\downarrow} - \mu) + (b^{\dagger}_{r\uparrow}b_{r\uparrow} - \mu)(b^{\dagger}_{r\downarrow}b_{r\downarrow} - \mu)], &(5)
\end{aligned}
$$

where r is a two-dimensional integral coordinate variable on each $L\times L$ lattice, δ is its nearest-neighbors on the plane. k is a two-dimensional integral momentum variable. q_z denotes the momentum perpendicular to the planes, the distance between which is $d = z_A - z_B$, where z_A and z_B are the vertical coordinates of the planes A and B, respectively. $a_{r\uparrow}$ and $a_{r\downarrow}$ are the coordinate-space annihilation operators for spin-up and spin-down electrons on layer A, respectively, $b_{r\uparrow}$ and $b_{r\downarrow}$ are those on layer B. $a_{k\uparrow}$, $a_{k\downarrow}$, $b_{k\uparrow}$ and $b_{k\downarrow}$ are the corresponding annihilation operators in the momentum space. μU is the chemical potential. $T_{\parallel}(A)$ and $T_{\parallel}(B)$ are kinetic energies on the two layers, respectively. $T_{\perp}$ is the interlayer coupling. V is the on-site electron-electron interaction potential energy. Following Ref. [3], we use

$$\epsilon(k) = 4 - 2\cos k_x - 2\cos k_y \tag{6}$$

to make the $T_{\|}(A)$ and $T_{\|}(B)$ positive. Actually as has been pointed out [3], only $\epsilon(k)+\epsilon(\pi-k) =$ constant is required to make η pairing possible.

For our present model, the operator η is introduced as

$$\eta \;=\; \eta_{\|}(A)+\eta_{\|}(B)+\eta_{\perp}, \tag{7}$$

with

$$\begin{aligned}\eta_{\|}(A) &= \sum_r e^{-i\pi\cdot r} a_{r\uparrow} a_{r\downarrow} \\ &= e^{2iq_z z_A} \sum_k a_{k\uparrow} a_{\pi-k\downarrow},\end{aligned} \tag{8}$$

$$\begin{aligned}\eta_{\|}(B) &= \sum_r e^{-i\pi\cdot r} b_{r\uparrow} b_{r\downarrow} \\ &= e^{2iq_z z_B} \sum_k b_{k\uparrow} b_{\pi-k\downarrow},\end{aligned} \tag{9}$$

and

$$\begin{aligned}\eta_{\perp} &= \sum_r e^{-i\pi\cdot r} (a_{r\uparrow} b_{r\downarrow} - a_{r\downarrow} b_{r\uparrow}) \\ &= e^{iq_z(z_A+z_B)} \sum_k (a_{k\uparrow} b_{\pi-k\downarrow} - a_{k\downarrow} b_{\pi-k\uparrow}),\end{aligned} \tag{10}$$

where π is two-dimensional. Actually $\eta_{\|}(A)$ and $\eta_{\|}(B)$ are on-site π-momentum pairings, while $\eta_{\perp}$ is the interlayer nearest-neighbor π-momentum pairing. The definition is, of course, only meaningful when L is even.

One can obtain the commutators

$$[T_{\|}(A)+T_{\|}(B),\, \eta_{\|}(A)+\eta_{\|}(B)] \;=\; -8t_{\|}[\eta_{\|}(A)+\eta_{\|}(B)], \tag{11}$$

$$[T_{\|}(A)+T_{\|}(B),\, \eta_{\perp}] \;=\; -8t_{\|}\eta_{\perp}, \tag{12}$$

$$[T_\perp,\, \eta_\parallel(A) + \eta_\parallel(B)] \;=\; -2t_\perp \eta_\perp, \tag{13}$$

$$[T_\perp,\, \eta_\perp] \;=\; -2t_\perp[\eta_\parallel(A) + \eta_\parallel(B)]. \tag{14}$$

Under the constraint condition

$$a^\dagger_{r\uparrow}a_{r\uparrow} + b^\dagger_{r\downarrow}b_{r\downarrow} \;=\; a^\dagger_{r\downarrow}a_{r\downarrow} + b^\dagger_{r\uparrow}b_{r\uparrow} \;=\; 1, \tag{15}$$

we may obtain

$$[V,\, \eta_\parallel(A) + \eta_\parallel(B)] \;=\; -(1-2\mu)U(\eta_\parallel(A) + \eta_\parallel(B)), \tag{16}$$

$$[V,\, \eta_\perp] \;=\; -(1-2\mu)U\eta_\perp. \tag{17}$$

Therefore under the constraint condition (15), we have

$$[H,\, \eta] \;=\; -E\eta, \tag{18}$$

where $E \;=\; 8t_\parallel + 2t_\perp + (1-2\mu)U$.

The total momentum operator P is

$$P \;=\; \sum_k (\mathbf{k} + \mathbf{q_z})(a^\dagger_{k\uparrow}a_{k\uparrow} + a^\dagger_{k\downarrow}a_{k\downarrow} + b^\dagger_{k\uparrow}b_{k\uparrow} + b^\dagger_{k\downarrow}b_{k\downarrow}), \tag{19}$$

the commutator of which with η is

$$[P,\, \eta] \;=\; -\pi\eta. \tag{20}$$

III. Eigenstates with ODLRO

We can generate the state

$$\psi_N \;=\; \beta(\eta^\dagger)^N|vac>, \tag{21}$$

where $|vac>$ is the vacuum state,

$$\beta = (N!(M-N)!/M!)^{1/2},\ M = L^2 \tag{22}$$

is the normalization factor. Because of (18) and (20), ψ_N is a simultaneous eigenstate of H and P,

$$H\psi_N = NE\psi_N, \tag{23}$$

$$P\psi_N = N\pi\psi_N. \tag{24}$$

Just similar to Ref. [3], one can construct another state ψ'_N, by replacing η in Eq. (21) with the 0-momentum pairing operator

$$\eta_0 = \sum_r (a_{r\uparrow}a_{r\downarrow} + b_{r\uparrow}b_{r\downarrow} + a_{r\uparrow}b_{r\downarrow} - a_{r\downarrow}b_{r\uparrow}). \tag{25}$$

ψ'_N has the same expectation value for H as ψ_N but is not an eigenstate. So ψ_N is not the ground state. Similar to Ref. [3], it can be proved to be metastable if $U < 0$.

Now we examine ODLRO. By definition, a state ψ possess ODLRO for a local operator Q_r means that the ODLRO correlation function

$$\lim_{|r-s|\to\infty} \psi^\dagger Q_s^\dagger Q_r \psi \neq 0. \tag{26}$$

In our system, there are three kinds of ODLRO correlation functions, the intralayer one for on-site pairing $\psi_N^\dagger a_{s\downarrow}^\dagger a_{s\uparrow}^\dagger a_{r\uparrow}a_{r\downarrow}\psi_N = \psi_N^\dagger b_{s\downarrow}^\dagger b_{s\uparrow}^\dagger b_{r\uparrow}b_{r\downarrow}\psi_N$, the interlayer one for on-site pairing $\psi_N^\dagger b_{s\downarrow}^\dagger b_{s\uparrow}^\dagger a_{r\uparrow}a_{r\downarrow}\psi_N = \psi_N^\dagger a_{s\downarrow}^\dagger a_{s\uparrow}^\dagger b_{r\uparrow}b_{r\downarrow}\psi_N$, and that for interlayer pairing $\psi_N^\dagger(b_{s\downarrow}^\dagger a_{s\uparrow}^\dagger - b_{s\uparrow}^\dagger a_{s\downarrow}^\dagger)(a_{r\uparrow}b_{r\downarrow} - a_{r\downarrow}b_{r\uparrow})\psi_N$, $r \neq s$. They all equal to

$$\frac{N(M-N)}{M(M-1)}e^{i\pi\cdot(r-s)}. \tag{27}$$

Therefore three kinds of ODLRO are simultaneously possessed by ψ_N.

IV. SO(4) symmetry

Define $\frac{\eta^\dagger}{2} = J_+ = J_x + iJ_y$, $\frac{\eta}{2} = J_- = J_x - iJ_y$, $J_z = \frac{1}{4}\sum_k (a^\dagger_{k\uparrow}a_{k\uparrow} + a^\dagger_{k\downarrow}a_{k\downarrow} + b^\dagger_{k\uparrow}b_{k\uparrow} + b^\dagger_{k\downarrow}b_{k\downarrow} + a^\dagger_{k\uparrow}b_{k\uparrow} + a^\dagger_{k\downarrow}b_{k\downarrow} + b^\dagger_{k\uparrow}a_{k\uparrow} + b^\dagger_{k\downarrow}a_{k\downarrow}) - \frac{M}{2}$. One may find that J_x, J_y and J_z are generators of an SU(2) symmetry. Under the constraint condition Eq. (15),

$$[H, J^2] = [H,\, J_z] = 0. \tag{28}$$

If the total momentum operator is trivially re-defined as

$$P' = \sum_k (\mathbf{k} - \frac{1}{2}\pi + \mathbf{q_z})(a^\dagger_{k\uparrow}a_{k\uparrow} + a^\dagger_{k\downarrow}a_{k\downarrow} + b^\dagger_{k\uparrow}b_{k\uparrow} + b^\dagger_{k\downarrow}b_{k\downarrow}), \tag{29}$$

we have

$$[P',\, \mathbf{J}] = 0. \tag{30}$$

From (18) we know that different from simple Hubbard model where $[H,\, \mathbf{J}] = 0$ [3], we cannot have $[H,\, \mathbf{J}] = 0$ for coupled bilayer even if we re-define $\epsilon(k)$ as $-2\cos k_x - 2\cos k_y$ and let $\mu = 1/2$, since $[T_\perp,\, \eta]$ cannot vanish.

The particle-hole pairing operator is

$$\zeta = \sum_r (a_{r\uparrow}a^\dagger_{r\downarrow} + b_{r\uparrow}b^\dagger_{r\downarrow}) = \sum_k (a_{k\uparrow}a^\dagger_{k\downarrow} + b_{k\uparrow}b^\dagger_{k\downarrow}). \tag{31}$$

Defining $\zeta^\dagger = J'_x + iJ'_y$, $\zeta = J'_x - J'_y$, $J'_z = \frac{1}{2}\sum_k (a^\dagger_{k\downarrow}a_{k\downarrow} + b^\dagger_{k\downarrow}b_{k\downarrow} - a^\dagger_{k\uparrow}a_{k\uparrow} - b^\dagger_{k\uparrow}b_{k\uparrow})$, one may find that J'_x, J'_y, J'_z are generators of an SU(2) symmetry, and that

$$[H,\, \mathbf{J}'] = [P',\, \mathbf{J}'] = 0. \tag{32}$$

Note that the constraint condition Eq. (15) is not required for Eq. (32), which just represents the SU(2) symmetry of spin.

Consequently, as in the simple Hubbard, there is also an SO(4) symmetry in the Hubbard bilayer, with the generators properly defined. Most of the discussions in Ref. [4] can thus generalized in a straightforward way, for example, many eigenfunctions for H and P' can be obtained explicitely, the symmetry properties of energy spectrum are almost also valid. One only needs to take into account that now there are two planes and the system is also symmetric under the exchange of the two planes.

However, the sufficient condition for a state to possess ODLRO should be reconsidered. It can be stated as follows.

Theorem. For any state ψ, if $j^2 - j_z^2 = O(M^2)$, where j and j_z are the quantum numbers of J^2 and J_z, respectively, then there is at least one kind of ODLRO among intralayer one for on-site pairing, interlayer one for on-site pairing and that for interlayer nearest-neighbor pairing.

Proof. Assume matrix Q has matrix element which is the ODLRO correlation function of the operator Δ,

$$Q_{sr} = < \Delta_r|Q|\Delta_s > = < \psi|\Delta_s^\dagger \Delta_r|\psi >, \tag{33}$$

Using

$$< \Delta_s|\phi > = M^{-1/2} e^{i\pi\cdot s} \tag{34}$$

as the trial wavefunction for Q, we obtain the expectation value of Q

$$< Q > = < \phi|Q|\phi > = \frac{1}{M} \sum e^{i\pi\cdot(s-r)} < \psi|\Delta_s^\dagger \Delta_r|\psi > . \tag{35}$$

On the other hand, we have

$$4(j^2 - j_z^2 + j + j_z) = < \psi|\eta^\dagger \eta|\psi > = \sum e^{i\pi\cdot(s-r)}(2Q_{sr}^{(1)} + 2Q_{sr}^{(2)} + Q_{sr}^{(3)}), \tag{36}$$

where

$$Q_{sr}^{(1)} = < \psi | a_{s\downarrow}^{\dagger} a_{s\uparrow}^{\dagger} a_{r\uparrow} a_{r\downarrow} | \psi > = < \psi | b_{s\downarrow}^{\dagger} b_{s\uparrow}^{\dagger} b_{r\uparrow} b_{r\downarrow} | \psi > \quad (37)$$

$$Q_{sr}^{(2)} = < \psi | a_{s\downarrow}^{\dagger} a_{s\uparrow}^{\dagger} b_{r\uparrow} b_{r\downarrow} | \psi > = < \psi | b_{s\downarrow}^{\dagger} b_{s\uparrow}^{\dagger} a_{r\uparrow} a_{r\downarrow} | \psi > \quad (38)$$

$$Q_{sr}^{(3)} = < \psi | (b_{s\downarrow}^{\dagger} a_{s\uparrow}^{\dagger} - b_{s\uparrow}^{\dagger} a_{s\downarrow})(a_{r\uparrow} b_{r\downarrow} - a_{r\downarrow} b_{r\uparrow}) | \psi > . \quad (39)$$

Therefore

$$2 < Q^{(1)} > + 2 < Q^{(2)} > + < Q^{(3)} > = \frac{1}{M}(j^2 - j_z^2) + O(1). \quad (40)$$

If $j^2 - j_z^2 = O(M^2)$, at least the largest of the eigenvalues of $Q^{(1)}$, $Q^{(2)}$ and $Q^{(3)}$ is O(M), according to Yang's Theorem [1], there is corresponding ODLRO. Q.E.D.

Tian proved a theorem that the ODLRO correlation function of a local operator R_r decays if there is another local operator S_r satisfying $[H, S_r] = R_r$ [9]. Using this theorem, we can obtain a useful result giving constraint on the ODLRO. By calculating $[H, \sum_r a_{r\uparrow} a_{\downarrow}]$, we know that $t_{\|} Q^{(nn)} + t_{\perp} Q^{(3)} - U(2\mu - 1) Q^{(1)}$ decays, here $Q^{(1)}$ and $Q^{(3)}$ are as defined above, $Q^{(nn)}$ is the ODLRO correlation function for intralayer nearest-neighbor s-wave pairing $\sum_{r,\delta}(a_{r\uparrow} a_{r+\delta\downarrow} - a_{r\downarrow} a_{r+\delta\uparrow})$. So the existence of one of the three ODLRO implies at least one of the other two. Furthermore, if $\mu = 1/2$, interlayer pairing ODLRO exists if and only if ODLRO for intralayer nearest-neighbor s-wave pairing exists. Consistent result has been obtained for the pairing amplitudes in the states with spontaneous gauge symmetry breaking [10].

V. Collective modes

In the Hubbard model, the SU(2) pseudospin symmetry contains the U(1) phase symmetry as a subgroup, whose spontaneously breaking, i.e., the superconductivity, gives rise to a pair of massive collective modes which together with the usual Goldstone mode form a triplet representation of the pseudospin symmetry [13]. Here we may see that these arguments can also extended to the bilayer model.

First it can be found that the operators $\Delta_- = \frac{1}{\sqrt{2}}\sum_r (a_{r\uparrow}a_{r\downarrow} + b_{r\uparrow}b_{r\downarrow} + a_{r\uparrow}b_{r\downarrow} - a_{r\downarrow}b_{r\uparrow})$, $\Delta_+ = -\Delta_-^\dagger$, and $\Delta_0 = \frac{1}{2}\sum_{r\sigma}(a^\dagger_{r\sigma}a_{r\sigma} + b^\dagger_{r\sigma}b_{r\sigma} + a^\dagger_{r\sigma}b_{r\sigma} + b^\dagger_{r\sigma}a_{r\sigma})$ form an irreducible tensor of rank 1 under the SU(2) defined by J_x, J_y and J_z in the last section. Then consider the response function

$$D_\alpha(t,t') = -\frac{i}{M}\theta(t-t') < [J_\alpha(t), \Delta_\alpha(t')] >, \tag{41}$$

where α denotes +, - or 0. One may obtain

$$D_0 = \frac{\rho}{\omega + i\delta}, \tag{42}$$

$$D_\pm(\omega) = \frac{< \Delta_\pm >}{\omega \pm E + i\delta}. \tag{43}$$

Therefore if the U(1) symmetry generated by J_z is spontaneously broken, i.e., if there is superconductivity with intralayer or(and) interlayer pairings, $< \Delta_+ > = - < \Delta_- >^* \neq 0$, then there is a triplet of collective modes with energies $\pm E$ and 0, respectively.

VI. Discussions

To summarize, by introducing an η operator generalized from Yang's and under a constraint condition, the discussions concerning ODLRO and SO(4) symmetry for simple Hubbard model are extended to Hubbard bilayer. In the explicitly constructed eigenstates, there are simultaneously three kinds of ODLRO, i.e., the intralayer one for on-site pairing, the interlayer one for on-site pairing, and that for interlayer nearest-neighbor pairing. By properly defining the generators, it is found that there is also an SO(4) symmetry. The sufficient condition for a state to possess ODLRO is that at least one of the three kinds of ODLRO exists if the condition is satisfied. We also obtain a constraint relation among the ODLRO for interlayer nearest-neighbor pairing, the intralayer ODLRO for on-site pairing, and that for intralayer s-wave nearest-neighbor pairing.

Though the explicit eigenstates possess the three kinds of ODLRO simultaneously, the sufficient condition can only ensure that at least one of them exsits. Another kind of ODLRO involves in the constraint relation. Further studies are needed to clarify whether these kinds of ODLRO must exist simultaneously.

Some exact results about the ground state of the simple Hubbard model are based on the exchange of η (pseudospin) and ζ (spin) operators under particle-hole transformation of the spin-up electrons [11] [12]. This situation is lost for the bilayer since the interlayer pairing is involved in our η operator.

Recently the collective modes predicted by Zhang [13] was generalized to the triplet case, which is then claimed to be responsible for the 41 meV peak in the

neutron scattering spectrum on YBa_2CuO_x [14]. However the dependence on q_z [5] could not be explained. Our results suggest that the bilayer model might be incorporated into the framework of this theory to account for the q_z dependence.

ACKNOWLEDGEMENT

R.B. Tao is acknowledged for helpful discussions.

References

[1] C. N. Yang, Rev. Mod. Phys. **34** (1962) 694.

[2] J. Bardeen, L. N. Cooper and J. R. Schrieffer, Phys. Rev. **108** (1987) 1175.

[3] C. N. Yang, Phys. Rev. Lett. **63** (1989) 2144.

[4] C. N. Yang and S. C. Zhang, Mod. Phys. Lett. B **4** (1990) 759.

[5] J. M. Tranquada *et al.*, Phys. Rev. B **46** (1992) 5561.

[6] J. Rossat-Mignod *et al.*, Physica B **180-181** (1992) 383.

[7] H. K. Mook *et al.*, Phys. Rev. Lett. **70** (1993) 3490.

[8] R. Stern *et al.*, Phys. Rev. B **50** (1994) 426.

[9] G. S. Tian, J. Phys. A **26** (1994) 2325.

[10] Y. Shi, Phys. Rev. B **51** (1995) 16619.

[11] E. H. Lieb, Phys. Rev. Lett. **62** (1989) 1201.

[12] S. Q. Shen and Z. M. Qiu, Phys. Rev. Lett. **71** (1993) 4238.

[13] S. C. Zhang, Phys. Rev. Lett. **65** (1990) 120.

[14] E. Demler and S. C. Zhang, Phys. Rev. Lett. **75** (1995) 4126.